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Semiclassical Approaches in Density Functional Theory PETER ELLIOTT, ATTILA CANGI, DONGHYUNG LEE, KIERON BURKE, University of California, Irvine — We discuss the use of semiclassical methods in understanding, and improving, density functional theory (DFT). It has been found[1] that semiclassical approaches can explain many features of modern exchange-correlation approximations, such as the local density approximation or generalized gradient approximations. In this work, we continue this line of inquiry, showing how semiclassical approximations may be used to construct a form for the non-interacting kinetic energy density. A semiclassical approximation to the Green's function is made[2], which, when integrated appropriately, yields leading corrections to the Thomas-Fermi result. It can be regarded as a functional of the potential. We test this approximation for various 1D systems confined within a box and present the results. This, coupled with the corresponding form of the density[2], could provide an orbital-free DFT which would allow more complex systems to be studied.
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[2] W. Kohn and L.J. Sham, Phys. Rev. **137**, A1697 (1965).

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